```
$%^STN; HighlightOn= ***; HighlightOff=*** ;
```

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:SSPTAPEZ1617

PASSW TERMI			ER 1	, 2, 3, OR ?):2
* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * * *
NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS	2	APR	04	STN AnaVist, Version 1, to be discontinued
NEWS	3	APR	15	WPIDS, WPINDEX, and WPIX enhanced with new
				predefined hit display formats
NEWS	4	APR	28	EMBASE Controlled Term thesaurus enhanced
NEWS	5	APR	28	IMSRESEARCH reloaded with enhancements
NEWS	6	MAY	30	INPAFAMDB now available on STN for patent family
				searching
NEWS	7	MAY	30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	8	JUN	0.6	EPFULL enhanced with 260,000 English abstracts
NEWS		JUN		KOREAPAT updated with 41,000 documents
NEWS		JUN		USPATFULL and USPAT2 updated with 11-character
MEMO	10	0.014	13	patent numbers for U.S. applications
NEWS	11	JUN	10	CAS REGISTRY includes selected substances from
MEMP	ΤI	JUN	19	web-based collections
NEWS	10	JUN	0.5	CA/CAplus and USPAT databases updated with IPC
MEMO	12	JUN	23	reclassification data
NEWS	1.0	7777	20	AEROSPACE enhanced with more than 1 million U.S.
NEWS	13	JUN	30	
NEWS	2.4	TIME	20	patent records
NEWS	14	JUN	30	EMBASE, EMBAL, and LEMBASE updated with additional
				options to display authors and affiliated
		****		organizations
NEWS	12	JUN	30	STN on the Web enhanced with new STN AnaVist
				Assistant and BLAST plug-in
NEWS		JUN		STN AnaVist enhanced with database content from EPFULL
NEWS		JUL		CA/CAplus patent coverage enhanced
NEWS	T.R	JUL	28	EPFULL enhanced with additional legal status
				information from the epoline Register
NEWS		JUL		IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS		JUL		STN Viewer performance improved
NEWS		AUG		INPADOCDB and INPAFAMDB coverage enhanced
NEWS	22	AUG	13	CA/CAplus enhanced with printed Chemical Abstracts
				page images from 1967-1998
NEWS		AUG		CAOLD to be discontinued on December 31, 2008
NEWS		AUG		CAplus currency for Korean patents enhanced
NEWS	25	AUG	25	CA/CAplus, CASREACT, and IFI and USPAT databases
				enhanced for more flexible patent number searching
NEWS	26	AUG	27	CAS definition of basic patents expanded to ensure

comprehensive access to substance and sequence

information

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 10:37:38 ON 08 SEP 2008

=> file rea

FULL ESTIMATED COST

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:37:51 ON 08 SEP 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\STNEXP\Queries\10542351.str

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR / Structure 1 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 10:38:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 105 TO ITERATE

100.0% PROCESSED 105 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 1486 TO 2714 PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss ful

FULL SEARCH INITIATED 10:38:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2279 TO ITERATE

100.0% PROCESSED 2279 ITERATIONS SEARCH TIME: 00.00.01 2 ANSWERS

L3 2 SEA SSS FUL L1

=> file cap

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 178.36 178.57

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 10:38:26 ON 08 SEP 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC)

reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 13 L4 2 L3

=> d 14 1-2 ibib abs hitstr

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:633527 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 141:174078

TITLE: Preparation of thienylpyridinecarbonitriles as bacterial enov1-ACP reductase (FabI) inhibitors.

INVENTOR(S): Moir, Donald T.; Xiang, Yibin; Arvanites, Anthony C.; Ali, Sved Masarrat; Geng, Bolin; Ashwell, Mark A.;

Orqueira, Hernan Antonio PATENT ASSIGNEE(S): Genome Therapeutics Corporation, USA; Argule

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGHAGE . English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO	٠.	KIN	D	DATE			APPLICATION NO.					DATE			
WO 200406	WO 2004064837					0805		WO 2004-US1327					20040116		
W: A	E, AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,
C	N, CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
G	E, GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	ΚZ,	LC,
L	K, LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ		
US 200700	A1 20070201				US 2006-542351					20060807					
PRIORITY APPLN					US 2003-441411P				1	P 20030117					
								WO 2	2004-	US13:	27	1	W 2	0040	116
OTHER SOURCE (S):	MARPAT 141:1740				78									

/ Structure 2 in file .gra /

GI

Title compds. I [R1, R2 = (un)substituted monocyclic arvl, heteroaryl; Y = X1-X2; X1 = bond, (un) substituted alkylene; X2 = aryl, heteroaryl, cycloaliph., etc.] and their pharmaceutically acceptable salts were prepd. For example, condensation-annulation of 1,3-di-2-thienyl-2-propen-1-one and 2-cyanoethanethioamide, followed by 4-(bromomethyl)benzoic acid S-alkylation of the resulting thioxopyridinecarbonitrile (no data provided), afforded claimed thienvlpyridinecarbonitrile II. In methicillin-resistant Staphylococcus aureus minimal inhibitory concn. (MIC) assays, 14-examples of compds. I exhibited MIC values ranging from 0.75->64 .mu.q/mL, e.g., the MIC value of thienvlpyridinecarbonitrile II

was 4 \dots mu.g/mL. Compds. I are claimed useful for the. Of note, compds. I are proposed to inhibit bacterial enoyl-ACP reductase (FabI), a NADH-dependent enoyl [acyl carrier protein] reductase enzyme in the fatty acid biosynthesis pathway.

T ***340808-61-9P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of thienylpyridinecarbonitriles as bacterial enoyl-ACP reductase (FabI) inhibitors.)

RN 340808-61-9 CAPLUS

CN Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA INDEX NAME)

/ Structure 3 in file .gra /

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:374624 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 141:239652

TITLE: Identification and characterization of inhibitors of bacterial enoyl-acyl carrier protein reductase

AUTHOR(S): Ling, Losee L.; Xian, Jun; Ali, Syed; Geng, Bolin; Fan, Jun; Mills, Debra M.; Arvanites, Anthony C.; Orqueira, Hernan; Ashwell, Mark A.; Carmel, Gilles;

Xiang, Yibin; Moir, Donald T.

CORPORATE SOURCE: Genome Therapeutics Corporation, Waltham, MA, 02453,

SOURCE: Antimicrobial Agents and Chemotherapy (2004), 48(5),

1541-1547

CODEN: AMACCQ; ISSN: 0066-4804 American Society for Microbiology

PUBLISHER: American
DOCUMENT TYPE: Journal
LANGUAGE: English

Bacterial enoyl-acyl carrier protein reductase (ENR) catalyzes an essential step in fatty acid biosynthesis. ENR is an attractive target for narrow-spectrum antibacterial drug discovery because of its essential role in metab, and its sequence conservation across many bacterial species. In addn., the bacterial ENR sequence and structural organization are distinctly different from those of mammalian fatty acid biosynthesis enzymes. High-throughput screening to identify inhibitors of Escherichia coli ENR yielded four structurally distinct classes of hits. Several members of one of these, the 2-(alkylthio)-4,6-diphenylpyridine-3carbonitriles ("thiopyridines"), inhibited both purified ENR (50% inhibitory concn. [IC50] = 3-25 .mu.M) and the growth of Staphylococcus aureus and Bacillus subtilis (MIC = 1-64 .mu.g/mL). The effect on cell growth is due in part to inhibition of fatty acid biosynthesis as judged by inhibition of incorporation of [14C] acetate into fatty acids and by the increased sensitivity of cells that underexpress an ENR-encoding gene (4-8-fold MIC shift). Synthesis of a variety of compds. in this chem. series revealed a correlation between IC50 and MIC, and the results provided initial structure-activity relationships. Preliminary structure-activity relationships, potency on purified ENR, and activity on bacterial cells indicate that members of the thiopyridine chem. series are

```
effective fatty acid biosynthesis inhibitors suitable for further
    antibacterial development.
      RL: BSU (Biological study, unclassified); BIOL (Biological study)
       (inhibitors of bacterial enoyl-acyl carrier protein reductase)
    340808-61-9 CAPLUS
RN
CN
    Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
    INDEX NAME)
/ Structure 4 in file .gra /
RN
    750595-50-7 CAPLUS
   Benzoic acid, 4-[1-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]-
    (CA INDEX NAME)
/ Structure 5 in file .gra /
REFERENCE COUNT:
                    26
                          THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
                           RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:v
COST IN U.S. DOLLARS
                                           SINCE FILE
                                                        TOTAL
                                                ENTRY SESSION
FULL ESTIMATED COST
                                                11.86
                                                       190.43
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                           SINCE FILE
                                                        TOTAL
                                               ENTRY SESSION
CA SUBSCRIBER PRICE
                                                -1.60
                                                         -1.60
STN INTERNATIONAL LOGOFF AT 10:39:35 ON 08 SEP 2008
Connecting via Winsock to STN
Welcome to STN International! Enter x:X
LOGINID: SSPTAPEZ1617
PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2
NEWS 1
               Web Page for STN Seminar Schedule - N. America
NEWS 2 APR 04 STN AnaVist, Version 1, to be discontinued
NEWS 3 APR 15 WPIDS, WPINDEX, and WPIX enhanced with new
               predefined hit display formats
```

```
NEWS 4 APR 28 EMBASE Controlled Term thesaurus enhanced
NEWS 5 APR 28 IMSRESEARCH reloaded with enhancements
NEWS 6 MAY 30 INPAFAMDB now available on STN for patent family
                searching
NEWS 7 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology
                sequence search option
NEWS 8 JUN 06 EPFULL enhanced with 260,000 English abstracts
NEWS 9 JUN 06 KOREAPAT updated with 41,000 documents
NEWS 10 JUN 13 USPATFULL and USPAT2 updated with 11-character
                patent numbers for U.S. applications
NEWS 11 JUN 19 CAS REGISTRY includes selected substances from
                web-based collections
NEWS 12 JUN 25 CA/CAplus and USPAT databases updated with IPC
                reclassification data
NEWS 13 JUN 30 AEROSPACE enhanced with more than 1 million U.S.
                patent records
NEWS 14 JUN 30 EMBASE, EMBAL, and LEMBASE updated with additional
                options to display authors and affiliated
                organizations
NEWS 15 JUN 30 STN on the Web enhanced with new STN AnaVist
                Assistant and BLAST plug-in
NEWS 16 JUN 30 STN AnaVist enhanced with database content from EPFULL
NEWS 17 JUL 28 CA/Caplus patent coverage enhanced
NEWS 18 JUL 28 EPFULL enhanced with additional legal status
                information from the epoline Register
NEWS 19 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 20 JUL 28 STN Viewer performance improved
NEWS 21 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced
NEWS 22 AUG 13 CA/CAplus enhanced with printed Chemical Abstracts
                page images from 1967-1998
NEWS 23 AUG 15 CAOLD to be discontinued on December 31, 2008
NEWS 24 AUG 15 CAplus currency for Korean patents enhanced
NEWS 25 AUG 25 CA/Caplus, CASREACT, and IFI and USPAT databases
                enhanced for more flexible patent number searching
NEWS 26 AUG 27 CAS definition of basic patents expanded to ensure
                comprehensive access to substance and sequence
                information
NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
```

AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability NEWS LOGIN Welcome Banner and News Items NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

result in loss of user privileges and other penalties.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may

=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.42 0.42

FILE 'REGISTRY' ENTERED AT 10:51:56 ON 08 SEP 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

 $\label{thm:c:program} {\tt Uploading C:\Program Files\STNEXP\Queries\10542351\ take\ 2.str}$

L1 STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS L1 STR / Structure 6 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 10:52:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 42 TO ITERATE

100.0% PROCESSED 42 ITERATIONS SEARCH TIME: 00.00.01 27 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 452 TO 1228
PROJECTED ANSWERS: 229 TO 851

=> s 11 sss ful

FULL SEARCH INITIATED 10:52:21 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 554 TO ITERATE

100.0% PROCESSED 554 ITERATIONS 342 ANSWERS

SEARCH TIME: 00.00.01

1.3 342 SEA SSS FUL L1

=> file cap

COST IN U.S. DOLLARS FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 178.36 178.78

FILE 'CAPLUS' ENTERED AT 10:52:26 ON 08 SEP 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 13

L4 5 T.3

=> d 14 1-5 ibib abs hitstr

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1016002 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 142:6311

TITLE: A preparation of benzamide derivatives, useful as

glyoxalase inhibitors

INVENTOR(S): Ashton, Mark; Davidson, Alan; Thomas, Russell;

Whittaker, Mark

PATENT ASSIGNEE(S): Chroma Therapeutics Limited, UK

SOURCE: PCT Int. Appl., 77 pp. CODEN: PIXXD2 Patent English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

DOCUMENT TYPE:

LANGUAGE:

PATENT NO. KIND DATE APPLICATION NO. DATE ----______ WO 2004101506 A1 20041125 WO 2004-GB2101 20040514 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG AU 2004238625 A1 20041125 AU 2004-238625 20040514 CA 2525438 A1 20041125 CA 2004-2525438 20040514 EP 1622869 20060208 EP 2004-733031 A1 20040514 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK JP 2006528964 T 20061228 JP 2006-530505 20040514 US 20070015799 A1 20070118 US 2005-556901 20051115 GB 2003-11195 A 20030515 WO 2004-GB2101 W 20040514 PRIORITY APPLN. INFO.: OTHER SOURCE(S): MARPAT 142:6311 GI

/ Structure 7 in file .gra /

AB The invention relates to a prepn. of benzamide derivs. of formula I [wherein: X is N or CH; RI is H, CN, halogen, NH2, or S-alkyl, etc.; R2 is H, CF3, (un)substituted aryl, cycloalkyl, or heterocyclyl, etc.; R3 is the same as R2 excluding CF3; R4 is H, (un)substituted aryl or heterocyclyl; R5 is H, (un)substituted alkyl, aryl, or alkylene-aryl; L1 is (un)substituted alkylene, arylene, or alkylene-arylene, etc.; L2 is a single bond, (un)substituted alkylene, or C(0)-alkylene, etc.; L3 and L4 are independently selected from a single bond, (un)substituted alkylene, or alkylene-wink(NGH)C(0)-arylene, etc.], useful as glyoxalase inhibitors. For instance, benzamide deriv. II (R6 = OR; 80% proliferation inhibition in H60s, IC50 = 8.3 nm.W) was prepd. via hydrolysis of N-(benzoyloxy)benzamide II [R6 = OC(0)Ph] with a yield of 41%.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzamide derivs. useful as glyoxalase inhibitors)

RN 354555-67-2 CAPLUS

CN Benzeneacetic acid, .alpha.-[(3-cyano-4,6-di-2-thieny1-2-pyridiny1)thio]-(CA INDEX NAME) / Structure 8 in file .gra /

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:633527 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 141:174078

TITLE: Preparation of thienylpyridinecarbonitriles as bacterial enoyl-ACF reductase (FabI) inhibitors.

INVENTOR(S): Moir, Donald T.; Xiang, Yibin; Arvanites, Anthony C.;
Ali, Syed Masarrat; Geng, Bolin; Ashwell, Mark A.;

Orgueira, Hernan Antonio

PATENT ASSIGNEE(S): Genome Therapeutics Corporation, USA; Arqule

SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATEN	IT NO.	KIN	D	DATE		APPLICATION NO.						DATE				
WO 20	A1 20040805			WO 2004-US1327						20040116						
T/	 AE, 	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ		
US 20	A1 20070201				US 2006-542351					20060807						
PRIORITY APPLN. INFO.:									US 2	003-	4414	11P	1	P 2	0030	117
									WO 2	004-	US13:	27	1	71 2	0040	116

OTHER SOURCE(S): MARPAT 141:174078

```
/ Structure 9 in file .gra /
```

AB Title compds. I [R1, R2 = (un)substituted monocyclic aryl, heteroaryl; Y = X1-X2; XI = bond, (un)substituted alkylene; X2 = aryl, heteroaryl, cycloaliph., etc.] and their pharmaceutically acceptable salts were prepd. For example, condensation-annulation of 1,3-di-2-thienyl-2-propen-1-one and 2-cyanoethanethioamide, followed by 4-(bromomethyl)benzoic acid S-alkylation of the resulting thioxopyridinecarbonitrile (no data provided), afforded claimed thienylpyridinecarbonitrile [II. In methicillin-resistant Staphylococcus aureus minimal inhibitory concn. (MIC) assays, 14-examples of compds. I exhibited MIC values ranging from 0.75->64.mu.g/ml, e.g., the MIC value of thienylpyridinecarbonitrile II was 4 mu.g/ml. Compds. I are claimed useful for the. Of note, compds. I are proposed to inhibit bacterial enoyl-ACP reductase (FabI), a NADH-dependent enoyl [acyl carrier protein] reductase enzyme in the fatty acid biosynthesis pathway.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

```
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. of thienvlpvridinecarbonitriles as bacterial enovl-ACP
        reductase (FabI) inhibitors.)
RN
     296797-06-3 CAPLUS
CN
    Acetamide, N-[3-(acetylamino)phenyl]-2-[(3-cyano-4,6-di-2-thienyl-2-
     pyridinyl)thio]- (CA INDEX NAME)
/ Structure 10 in file .gra /
RN
     340808-61-9 CAPLUS
     Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
     INDEX NAME)
/ Structure 11 in file .gra /
     354555-67-2 CAPLUS
RN
     Benzeneacetic acid, .alpha.-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]-
     (CA INDEX NAME)
/ Structure 12 in file .gra /
     733052-04-5 CAPLUS
RN
CN
     Benzoic acid, 4-[2-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]-
     (CA INDEX NAME)
/ Structure 13 in file .gra /
     733052-05-6 CAPLUS
RN
CN
     3-Pyridinecarbonitrile, 2-[(1-phenylethyl)thio]-4,6-di-2-thienyl- (CA
     INDEX NAME)
/ Structure 14 in file .gra /
RN
     733052-06-7 CAPLUS
CN
     Benzoic acid, 3-[[(3-cvano-4,6-di-2-thienvl-2-pvridinvl)thio]methvl]- (CA
     INDEX NAME)
/ Structure 15 in file .gra /
RM
     733052-07-8 CAPLUS
CN
     Benzeneacetic acid, 4-[[(3-cvano-4,6-di-2-thienvl-2-pyridinvl)thio]methyl]-
       (CA INDEX NAME)
/ Structure 16 in file .gra /
BM
     733052-09-0 CAPLUS
     Propanoic acid, 3-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]- (CA INDEX
     NAME)
```

```
/ Structure 17 in file .gra /
```

IT ***243987-05-5P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of thienylpyridinecarbonitriles as bacterial enoyl-ACP reductase (FabI) inhibitors.)

RN 243987-05-5 CAPLUS

CN 3-Pyridinecarbonitrile, 1,2-dihydro-4,6-di-2-thienyl-2-thioxo- (CA INDEX NAME)

/ Structure 18 in file .gra /

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RECORD. AND CITATIONS AVAIDABLE IN THE RE

L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:374624 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 141:239652

TITLE: Identification and characterization of inhibitors of bacterial enovl-acyl carrier protein reductase

AUTHOR(S): Ling, Losee L.; Xian, Jun; Alī, Syed; Geng, Bolin; Fan, Jun; Mills, Debra M.; Arvanites, Anthony C.; Orqueira, Hernan; Rahwell, Mark A.; Carmel, Gilles;

Xiang, Yibin: Moir, Donald T.

CORPORATE SOURCE: Genome Therapeutics Corporation, Waltham, MA, 02453,

USA

SOURCE: Antimicrobial Agents and Chemotherapy (2004), 48(5),

1541-1547

CODEN: AMACCQ; ISSN: 0066-4804

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal

antibacterial development.

LANGUAGE: English Bacterial enov1-acv1 carrier protein reductase (ENR) catalyzes an essential step in fatty acid biosynthesis. ENR is an attractive target for narrow-spectrum antibacterial drug discovery because of its essential role in metab. and its sequence conservation across many bacterial species. In addn., the bacterial ENR sequence and structural organization are distinctly different from those of mammalian fatty acid biosynthesis enzymes. High-throughput screening to identify inhibitors of Escherichia coli ENR yielded four structurally distinct classes of hits. Several members of one of these, the 2-(alkylthio)-4,6-diphenylpyridine-3carbonitriles ("thiopyridines"), inhibited both purified ENR (50% inhibitory concn. [IC50] = 3-25 .mu.M) and the growth of Staphylococcus aureus and Bacillus subtilis (MIC = 1-64 .mu.g/mL). The effect on cell growth is due in part to inhibition of fatty acid biosynthesis as judged by inhibition of incorporation of [14C] acetate into fatty acids and by the increased sensitivity of cells that underexpress an ENR-encoding gene (4-8-fold MIC shift). Synthesis of a variety of compds. in this chem. series revealed a correlation between IC50 and MIC, and the results provided initial structure-activity relationships. Preliminary structure-activity relationships, potency on purified ENR, and activity on bacterial cells indicate that members of the thiopyridine chem. series are effective fatty acid biosynthesis inhibitors suitable for further

```
ТТ
     , GTC 343130 ***733052-07-8*** , GTC 330346
      ***733052-06-7***
      ***750595-50-7*** , GTC 343131
    RL: BSU (Biological study, unclassified); BIOL (Biological study)
       (inhibitors of bacterial enoyl-acyl carrier protein reductase)
RN
    296797-06-3 CAPLUS
CN Acetamide, N-[3-(acetvlamino)phenvl]-2-[(3-cvano-4,6-di-2-thienvl-2-
    pyridinyl)thio]- (CA INDEX NAME)
/ Structure 19 in file .gra /
    340808-61-9 CAPLUS
CN Benzoic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
    INDEX NAME)
/ Structure 20 in file .gra /
    354555-67-2 CAPLUS
   Benzeneacetic acid, .alpha.-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]-
CN
    (CA INDEX NAME)
/ Structure 21 in file .gra /
    733052-04-5 CAPLUS
RN
    Benzoic acid, 4-[2-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]-
CN
    (CA INDEX NAME)
/ Structure 22 in file .gra /
    733052-06-7 CAPLUS
    Benzoic acid, 3-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]- (CA
CN
    INDEX NAME)
/ Structure 23 in file .gra /
RN
    733052-07-8 CAPLUS
CN
    Benzeneacetic acid, 4-[[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]methyl]-
      (CA INDEX NAME)
/ Structure 24 in file .gra /
    750595-50-7 CAPLUS
CN Benzoic acid, 4-[1-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]ethyl]-
    (CA INDEX NAME)
/ Structure 25 in file .gra /
REFERENCE COUNT:
                     26
                           THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
                           RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
```

```
L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         2000:412595 CAPLUS << LOGINID::20080908>>
DOCUMENT NUMBER:
                         133:207831
TITLE:
                         Synthesis of substituted 4-hydroxy-1H-thieno(2,3-b;4,5-
                         b']dipyridin-2-ones
AUTHOR(S):
                         Rodinovskaya, L. A.; Shestopalov, A. M.
CORPORATE SOURCE:
                         N. D. Zelinsky Institute of Organic Chemistry, Russian
                         Academy of Sciences, Moscow, 117913, Russia
SOURCE:
                         Russian Chemical Bulletin (Translation of Izvestiva
                         Akademii Nauk, Seriya Khimicheskaya) (2000), 49(2),
                         348-354
                         CODEN: RCBUEY; ISSN: 1066-5285
PUBLISHER:
                         Consultants Bureau
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
GT
/ Structure 26 in file .gra /
AR
     Substituted 4-hydroxy-1H-thieno[2,3-b;4,5-b']dipyridin-2-ones, e.g., I,
     were prepd. by reaction of 3-cyanopyridine-2(1H)-thiones with alkyl
     4-chloroacetoacetates and by intramol. cyclization of alkyl
     4-(2-pyridylthio)acetoacetates or alkyl 3-(3-aminothieno[2,3-b]pyridin-2-
     yl)-3-oxopropionates under the action of bases.
       ***243987-05-5***
TT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of 4-hydroxy-1H-thieno[2,3-b;4,5-b']dipyridin-2-ones)
     243987-05-5 CAPLUS
CN
     3-Pyridinecarbonitrile, 1,2-dihydro-4,6-di-2-thienyl-2-thioxo- (CA INDEX
     NAME)
/ Structure 27 in file .gra /
       ***290299-69-3P***
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of 4-hvdroxv-1H-thieno[2,3-b;4,5-b'ldipvridin-2-ones)
RN
     290299-69-3 CAPLUS
CN
     Butanoic acid, 4-[(3-cyano-4,6-di-2-thienyl-2-pyridinyl)thio]-3-oxo-,
     ethyl ester (CA INDEX NAME)
/ Structure 28 in file .gra /
REFERENCE COUNT:
                        9
                               THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
    ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
                        1999:455705 CAPLUS <<LOGINID::20080908>>
ACCESSION NUMBER:
DOCUMENT NUMBER:
                        131:228634
TITLE:
                         One stage synthesis of 4,6-diary1-3-cyanopyridine-
                        2(1H)-thiones
AUTHOR(S):
                        Shestopalov, A. M.; Nikishin, K. G.
```

CORPORATE SOURCE: N. D. Zelinskii Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 117913, Russia

SOURCE: Chemistry of Heterocyclic Compounds (New

> York) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (1999), Volume Date 1998, 34(9), 1093

> > -4.00

-4.00

CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

The title compds. were prepd. in 82-92% yields by cyclization of .alpha., .beta.-unsatd. ketones with malononitrile and S in refluxing EtOH in the presence of morpholine.

243987-05-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of diarylcvanopyridine 2(1H)-thiones)

RN 243987-05-5 CAPLUS

3-Pvridinecarbonitrile, 1,2-dihvdro-4,6-di-2-thienvl-2-thioxo- (CA INDEX NAME)

/ Structure 29 in file .gra /

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file stng

COST IN U.S. DOLLARS SINCE FILE TOTAL. ENTRY SESSION FULL ESTIMATED COST 28.21 206.99 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL. ENTRY SESSION

FILE 'STNGUIDE' ENTERED AT 10:53:52 ON 08 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Sep 5, 2008 (20080905/UP).

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:v

CA SUBSCRIBER PRICE

COST IN U.S. DOLLARS SINCE FILE TOTAL. ENTRY SESSION FULL ESTIMATED COST 1.26 208.25 DISCOUNT AMOUNTS (FOR OUALIFYING ACCOUNTS) SINCE FILE TOTAL SESSION ENTRY CA SUBSCRIBER PRICE 0.00 -4.00

STN INTERNATIONAL LOGOFF AT 11:06:18 ON 08 SEP 2008

Welcome to STN International! Enter x:X LOGINID:SSPTAPEZ1617 PASSWORD: TERMINAL (ENTER 1, 2, 3, OR ?):2 * * * * * * * * * * Welcome to STN International * * * * * * * * * NEWS 1 Web Page for STN Seminar Schedule - N. America NEWS 2 APR 04 STN AnaVist, Version 1, to be discontinued NEWS 3 APR 15 WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats NEWS 4 APR 28 EMBASE Controlled Term thesaurus enhanced NEWS 5 APR 28 IMSRESEARCH reloaded with enhancements NEWS 6 MAY 30 INPAFAMDB now available on STN for patent family searching NEWS 7 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option NEWS 8 JUN 06 EPFULL enhanced with 260,000 English abstracts NEWS 9 JUN 06 KOREAPAT updated with 41,000 documents NEWS 10 JUN 13 USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications NEWS 11 JUN 19 CAS REGISTRY includes selected substances from web-based collections NEWS 12 JUN 25 CA/CAplus and USPAT databases updated with IPC reclassification data NEWS 13 JUN 30 AEROSPACE enhanced with more than 1 million U.S. patent records NEWS 14 JUN 30 EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations NEWS 15 JUN 30 STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in NEWS 16 JUN 30 STN AnaVist enhanced with database content from EPFULL NEWS 17 JUL 28 CA/CAplus patent coverage enhanced NEWS 18 JUL 28 EPFULL enhanced with additional legal status information from the epoline Register NEWS 19 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements NEWS 20 JUL 28 STN Viewer performance improved NEWS 21 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced NEWS 22 AUG 13 CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998 NEWS 23 AUG 15 CAOLD to be discontinued on December 31, 2008 NEWS 24 AUG 15 Caplus currency for Korean patents enhanced NEWS 25 AUG 25 CA/Caplus, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching

NEWS 26 AUG 27 CAS definition of basic patents expanded to ensure

information

comprehensive access to substance and sequence

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 11:31:17 ON 08 SEP 2008

=>

Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):

Switching to the Registry File ...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 11:31:41 ON 08 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by ${\tt InfoChem.}$

STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of

```
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:
http://www.cas.org/support/stngen/stndoc/properties.html
=>
Uploading C:\Program Files\STNEXP\Queries\10542351 take 3.str
L1 STRUCTURE UPLOADED
=> d 11
L1 HAS NO ANSWERS
L1
/ Structure 30 in file .gra /
Structure attributes must be viewed using STN Express query preparation.
Uploading C:\Program Files\STNEXP\Oueries\10542351 take 4.str
L2 STRUCTURE UPLOADED
=> d 12
L2 HAS NO ANSWERS
L2
/ Structure 31 in file .gra /
Structure attributes must be viewed using STN Express query preparation.
=> s 11 or 12
SAMPLE SEARCH INITIATED 11:32:19 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                   646 TO ITERATE
100.0% PROCESSED 646 ITERATIONS
                                                             11 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS: 11396 TO 14444
PROJECTED ANSWERS:
                              22 TO
                                       418
L3
           11 SEA SSS SAM L1 OR L2
=> s 11 sss full
FULL SEARCH INITIATED 11:32:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 18549 TO ITERATE
100.0% PROCESSED 18549 ITERATIONS
                                                            285 ANSWERS
SEARCH TIME: 00.00.01
L4 285 SEA SSS FUL L1
```

=> s 12 sss ful FULL SEARCH INITIATED 11:32:33 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 742 TO ITERATE

100.0% PROCESSED 742 ITERATIONS 2 ANSWERS

SEARCH TIME: 00.00.01

1.5 2 SEA SSS FUL L2

=> file cap

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 356.72 356.93

FILE 'CAPLUS' ENTERED AT 11:32:42 ON 08 SEP 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 14 or 15 100 T.4

3 L5 102 L4 OR L5

1.6

=> s 16 and bacteria

348391 BACTERIA 129 BACTERIAS

348461 BACTERIA

(BACTERIA OR BACTERIAS)

3 L6 AND BACTERIA

=> d 1-3 17 ibib abs hitstr

L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:196524 CAPLUS <<LOGINID::20080908>>

```
DOCUMENT NUMBER:
                        147 - 419384
TITLE:
                        New antimicrobial 9-(p-heterocyclo-substituted
                         anilino)-tetrahvdroacridines
                         Ebeid, M. Y.; Kamel, M. M.; Nofal, Z. M.; Ragab, F.;
AUTHOR(S):
                         Zaghary, W. A.; El-Kady, M.
CORPORATE SOURCE:
                         Faculty of Pharmacy, Cairo University, Egypt
SOURCE:
                         Egyptian Journal of Chemistry (2006), 49(2), 277-285
                         CODEN: EGJCA3; ISSN: 0449-2285
PUBLISHER:
                         National Information and Documentation Centre
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
   A new series of 9-[p-(4-aryl-3-cyano-2-iminopyridin-6-yl)anilino]-
     1,2,3,4-tetrahydroacridines and their 2-oxo-(or thioxo)-pyridinylanilino
     derivs. were synthesized and evaluated against
                                                     ***bacteria***
     fungi. These compds. showed high significant activity against
     Saccharomyces cerevisiae, Bacillus subtilis, Staphylococcus aureus,
     Penicillium notatum, Aspergillus niger, Candida utilis, and Candida
     albicans.
TТ
      ***951320-46-0P***
     RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation)
        (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahvdroacridines)
RN
     951320-46-0 CAPLUS
CN
    3-Pyridinecarbonitrile, 1,2-dihydro-4-phenyl-6-[4-[(1,2,3,4-tetrahydro-9-
     acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 32 in file .gra /
       ***951320-47-1P***
                            ***951320-48-2P***
                                                    ***951320-49-3P***
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
        (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahydroacridines)
RN
     951320-47-1 CAPLUS
     3-Pyridinecarbonitrile, 1, 2-dihydro-4-(3-methoxypheny1)-6-[4-[(1, 2, 3, 4-
CN
     tetrahydro-9-acridinyl)aminolphenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 33 in file .gra /
     951320-48-2 CAPLUS
CN
   3-Pyridinecarbonitrile, 4-(3-chlorophenyl)-1,2-dihydro-6-[4-[(1,2,3,4-
     tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 34 in file .gra /
     951320-49-3 CAPLUS
     3-Pyridinecarbonitrile, 1,2-dihydro-6-[4-[(1,2,3,4-tetrahydro-9-
     acridinyl)amino]phenyl]-2-thioxo-4-(2,3,4-trimethoxyphenyl)- (CA INDEX
     NAME)
/ Structure 35 in file .gra /
TT
     ***951320-50-6***
```

```
RL: RCT (Reactant); RACT (Reactant or reagent)
        (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahvdroacridines)
RN
     951320-50-6 CAPLUS
CN
     3-Pyridinecarbonitrile, 4-[3-(dimethylamino)phenyl]-1,2-dihydro-6-[4-
     [(1,2,3,4-tetrahydro-9-acridiny1)amino]pheny1]-2-thioxo- (CA INDEX NAME)
/ Structure 36 in file .gra /
REFERENCE COUNT:
                        20
                               THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT
L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1999:221628 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         130:325083
TITLE:
                         Synthesis and antimicrobial activity of some new
                         4-methylquinolines
AUTHOR(S):
                         Kamel, M. M.; Fathala, O. A.; Abdou, W. A. M.; Haiba,
                         M. E.
CORPORATE SOURCE:
                         Medicinal Chemistry Department, National Research
                         Centre, Cairo, Egypt
SOURCE:
                         Proceedings of the Pakistan Academy of Sciences
                         (1997), 34(1), 7-11
                         CODEN: PKSPAW; ISSN: 0377-2969
PUBLISHER:
                         Pakistan Academy of Sciences
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     Some new 4,8-dimethyl-2-[p-(3-cyano-2-thioxo-4-arylpyridine-6-
     v1) lanilinoquinolines and 7-chloro-4-methv1-2-(4-hvdroxy)anilinoquinoline
     Mannich bases were synthesized for the purpose of antimicrobial evaluation
              ***bacteria*** , yeast, and fungi. Two compds. showed activity
     against
     against these microorganisms.
                                                   ***218272-69-6P***
       ***218272-67-4P***
                             ***218272-68-5P***
       ***223697-02-7P***
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of methylquinolines as antibacterial and antifungal agents)
RN
     218272-67-4 CAPLUS
CN
     3-Pvridinecarbonitrile, 6-[4-[(4,8-dimethvl-2-quinolinvl)aminolphenvl]-1,2-
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 37 in file .gra /
RM
     218272-68-5 CAPLUS
     3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-6-[4-[(4,8-dimethyl-2-
     quinoliny1)amino]pheny1]-1,2-dihydro-2-thioxo- (CA INDEX NAME)
/ Structure 38 in file .gra /
BM
     218272-69-6 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
CN
```

dihydro-4-(3-methoxy-2-nitropheny1)-2-thioxo- (CA INDEX NAME)

```
/ Structure 39 in file .gra /
     223697-02-7 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(7-chloro-4-methyl-2-
     quinolinyl)amino[phenyl]-1,2-dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA
     INDEX NAME)
/ Structure 40 in file .gra /
                               THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         17
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         1998:702455 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         130:66375
TITLE:
                         Synthesis of some new 4-methylquinolines of possible
                         biological activity
AUTHOR(S):
                         Kamel, M. M.; Fathalla, O. A.; Abdou, W. A. M.; Omer,
                         M. T.; Haiba, M. E.
CORPORATE SOURCE:
                         Medicinal Chemistry Department, National Research
                         Centre, Cairo, Egypt
SOURCE:
                         Egyptian Journal of Pharmaceutical Sciences (1998),
                         Volume Date 1997, 38(1-3), 79-86
                         CODEN: EJPSBZ; ISSN: 0301-5068
PUBLISHER:
                         National Information and Documentation Centre
DOCUMENT TYPE:
                         Journal.
LANGUAGE:
                         English
     Some new 4,8-dimethyl-2-[p-(3-cvano-2-thioxo-4-arylpyridin-6-
     yl)]anilinoquinolines and 7-chloro-4-methyl-2-(4-hydroxy)anilinoquinolines
     Mannich bases were synthesized for the purpose of antimicrobial evaluation
     against ***bacteria*** , yeast, and fungi. 7-Chloro-4-methyl-2-[4-
     hydroxy-3,5-di(diethylaminomethyl)]anilinoquinoline showed fungicidal
     activity against Aspergillus niger.
       ***218272-67-4P***
                            ***218272-68-5P***
                                                    ***218272-69-6P***
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis and antimicrobial activity of 4-methylquinolines)
RN
     218272-67-4 CAPLUS
CN
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 41 in file .gra /
DM
     218272-68-5 CAPLUS
CN
     3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-6-[4-[(4,8-dimethyl-2-
     quinolinvl)aminolphenvl]-1,2-dihvdro-2-thioxo- (CA INDEX NAME)
/ Structure 42 in file .gra /
     218272-69-6 CAPLUS
DM
CN
     3-Pyridinecarbonitrile, 6-[4-[(4.8-dimethyl-2-guinolinyl)aminolphenyl]-1,2-
     dihydro-4-(3-methoxy-2-nitrophenyl)-2-thioxo- (CA INDEX NAME)
```

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file stng
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTINATED COST 21.83 378.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL
ENTRY SESSION
CA SUBSCRIBER PRICE -2.40 -2.40

FILE 'STNGUIDE' ENTERED AT 11:36:57 ON 08 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Sep 5, 2008 (20080905/UP).

=> file stng
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 0.66 379.42

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | ENTRY | SESSION | CA SUBSCRIBER PRICE | 0.00 | -2.40

FILE 'STNGUIDE' ENTERED AT 11:43:28 ON 08 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Sep 5, 2008 (20080905/UP).

CA SUBSCRIBER PRICE

=> file reg
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
ENTRY SESSION
ENTRY SESSION
ENTRY SESSION

0.00

-2.40

FILE 'REGISTRY' ENTERED AT 11:48:40 ON 08 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by ${\tt InfoChem.}$

STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=

Uploading C:\Program Files\STNEXP\Queries\10542351 take 5.str

L8 STRUCTURE UPLOADED

=> d 18

L8 HAS NO ANSWERS L8 STR

/ Structure 44 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 18 sss ful

FULL SEARCH INITIATED 11:49:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1468 TO ITERATE

100.0% PROCESSED 1468 ITERATIONS SEARCH TIME: 00.00.01 16 ANSWERS

-2.40

0.00

DEFINCT TIME: 00.00.01

CA SUBSCRIBER PRICE

L9 16 SEA SSS FUL L8

=> file cap

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 178.36 558.32 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

FILE 'CAPLUS' ENTERED AT 11:49:09 ON 08 SEP 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December

26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 19 L10 5 L9

=> d 110 1-5 ibib abs hitstf
'HITSTF' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations

The following are valid formats:

ABS ----- GI and AB

```
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
             SCAN must be entered on the same line as the DISPLAY,
             e.g., D SCAN or DISPLAY SCAN)
STD ---- BIB, CLASS
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
```

SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms

HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)

containing hit terms

HITRN ----- HIT RN and its text modification

HITSTR ----- HIT RN, its text modification, its CA index name, and

its structure diagram

HITSEQ ----- HIT RN, its text modification, its CA index name, its

structure diagram, plus NTE and SEQ fields

FHITSTR ---- First HIT RN, its text modification, its CA index name, and

its structure diagram FHITSEQ ---- First HIT RN, its text modification, its CA index name, its

structure diagram, plus NTE and SEQ fields

KWIC ----- Hit term plus 20 words on either side

OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI, IND; TI, SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number. ENTER DISPLAY FORMAT (BIB):end

=> d 110 1-5 ibib abs hitstr

AUTHOR(S):

L10 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:798258 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 148:538031

TITLE: Synthesis and investigation of the stability of esters of 6'-carbamoylmethylthio-5'-cyano-1', 4'-dihydro-3, 4'-

and -4,4'-bipyridine-3'-carboxylic acids. Part 1. Esters of 6'-carbamoylmethylthio-5'-cyano-1',4'dihydro-3,4'-bipyridine-3'-carboxylic acids

Kazoka, H.; Krauze, A.; Vilums, M.; Cernova, L.; Sile,

L.; Duburs, G.

CORPORATE SOURCE: Latvian Institute of Organic Synthesis, Riga, LV-1006,

Latvia

SOURCE: Chemistry of Heterocyclic Compounds (New York, NY,

United States) (2007), 43(1), 50-57

CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Springer

DOCUMENT TYPE: Journal LANGUAGE: English

Esters of 6'-carbamoylmethylthio-5'-cyano-1',4'-dihydro-3,4'-bipyridine-3'carboxylic acids are obtained by the alkylation of piperidinium 3'-alkoxycarbonyl-5'-cyano-1',4'-dihydro-3,4'-bipyridine-6'-thiolates with iodoacetamide. For an HPLC study of the stability of solns. of the abovementioned 1.4-dihydrobipyridines (soln., pH 2.3-9.0), the appropriate esters of 6'-carbamoylmethylthio-5'-cyano-3,4'-bipyridine-3'-carboxylic acids and esters of 8-cyano-5-methyl(or phenyl)-3-oxo-7-pyridin-3-yl-2,3dihydro-7H-thiazolo[3,2-a]pyridine-6-carboxylic acids were synthesized as

reverse-phase chromatog. It was shown that solns. of the investigated compds. in a mixt. of MeCN and phosphate buffer (pH 3.0-5.0) were stable for 1 mo on storage protected from light. Under the action of light in all the solns, investigated irresp, of pH, the formation occurs of the corresponding esters of 6'-carbamoylmethylthio-5'-cyano-3,4'-bipyridine-3'carboxylic acids. The presence of esters of 8-cyano-5-methyl(or phenv1)-3-oxo-7-pyridin-3-v1-2,3-dihydro-7H-thiazolo[3,2-a]pyridine-6carboxylic acids (.ltoreq.4%) was detected only in 0.1% solns. of phosphoric acid (pH 2.3) under conditions of storage of the latter protected from light. A series of as yet unidentified products was detected in solns. of pH 7.0-9.0. ***144969-93-7P*** RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and stability of esters of (carbamoylmethylthio)cyanodihydrobip vridinecarboxvlates) 144969-93-7 CAPLUS [3,4'-Bipyridine]-3'-carboxylic acid, 6'-[(2-amino-2-oxoethyl)thio]-5'cvano-2'-phenvl-, ethvl ester (CA INDEX NAME) / Structure 45 in file .gra / REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT L10 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1999:547305 CAPLUS <<LOGINID::20080908>> 131:295109 DOCUMENT NUMBER: TITLE: Derivatives of 3-cvano-6-phenvl-4-(3'-pvridvl)pyridine-2(1H)-thione and their neurotropic activity Krauze, Aivars; Germane, Skaidrite; Eberlins, Ojars; AUTHOR(S): Sturms, Igors; Klusa, Vija; Duburs, Gunars CORPORATE SOURCE: Latvian Institute of Organic Synthesis, Riga, LV-1006, Latvia European Journal of Medicinal Chemistry (1999), 34(4), SOURCE: 301-310 CODEN: EJMCA5: ISSN: 0223-5234 PUBLISHER: Editions Scientifiques et Medicales Elsevier DOCUMENT TYPE: Journal LANGUAGE: English 3-Cyano-6-phenyl-4-(3'-pyridyl)pyridine-2(1H)-thione, the related 2,2'-bis-pyridyldisulfide, 2-alkylthiopyridines and 2-amino-thieno[2,3b]pyridines were synthesized and their neurotropic activities were examd. Bispyridyldisulfide exhibited low toxicity (LD50 > 5000 mg/kg, ICR mice, i.p.) and selective antiamnesic activity at the doses of 0.05-0.5 mg/kg p.o. This effect was significantly higher than that induced by Piracetam at 50 mg/kg. ***247056-20-8P*** ***247056-23-1P*** ***247056-24-2P*** ***247056-25-3P*** ***247056-26-4P*** ***247056-27-5P*** ***247056-28-6P*** RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. and neurotropic activity of 3-cyano-6-phenyl-4-(3'-pyridyl)-

ref. compds. Anal. by HPLC was carried out under conditions of

RN

CN

ΙT

pyridine-2(1H)-thione derivs.)

```
RN
    247056-20-8 CAPLUS
CN
    [3,4'-Bipyridine]-3'-carbonitrile, 1',2'-dihydro-6'-phenyl-2'-thioxo- (CA
     INDEX NAME)
/ Structure 46 in file .gra /
    247056-23-1 CAPLUS
RN
    [3,4'-Bipyridine]-3'-carbonitrile, 2'-(methylthio)-6'-phenyl- (CA INDEX
CN
    NAME)
/ Structure 47 in file .gra /
DM
     247056-24-2 CAPLUS
    [3,4'-Bipyridine]-3'-carbonitrile, 2'-(ethylthio)-6'-phenyl- (CA INDEX
CN
    NAME)
/ Structure 48 in file .gra /
    247056-25-3 CAPLUS
RN
CN
    Acetic acid, 2-[(3'-cvano-6'-phenyl[3,4'-bipyridin]-2'-vl)thio]-, ethyl
    ester (CA INDEX NAME)
/ Structure 49 in file .gra /
RN
     247056-26-4 CAPLUS
CN
    [3,4'-Bipyridine]-3'-carbonitrile, 2'-[(cvanomethyl)thio]-6'-phenyl- (CA
     INDEX NAME)
/ Structure 50 in file .gra /
    247056-27-5 CAPLUS
BM
    Acetamide, 2-[(3'-cyano-6'-phenyl[3,4'-bipyridin]-2'-yl)thio]- (CA INDEX
CN
/ Structure 51 in file .gra /
     247056-28-6 CAPLUS
RN
     [3,4'-Bipyridine]-3'-carbonitrile, 2'-[(2-oxo-2-phenylethyl)thio]-6'-
     phenyl- (CA INDEX NAME)
/ Structure 52 in file .gra /
TТ
      ***247056-21-9P***
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (prepn. and neurotropic activity of 3-cyano-6-phenyl-4-(3'-pyridyl)-
        pyridine-2(1H)-thione derivs.)
   247056-21-9 CAPLUS
RN
```

```
[3,4'-Bipyridine]-3'-carbonitrile, 2',2'''-dithiobis[6'-phenyl- (9CI) (CA
     INDEX NAME)
/ Structure 53 in file .gra /
ΙT
       ***247056-22-0P***
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and neurotropic activity of 3-cyano-6-phenyl-4-(3'-pyridyl)-
        pyridine-2(1H)-thione derivs.)
RN
     247056-22-0 CAPLUS
CN
    [3,4'-Bipyridine]-3'-carbonitrile, 6'-phenyl-2'-(1-piperidinylthio)- (CA
     INDEX NAME)
/ Structure 54 in file .gra /
REFERENCE COUNT:
                         48
                              THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L10 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1993:38791 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         118:38791
ORIGINAL REFERENCE NO.: 118:7067a,7070a
TITLE .
                        Synthesis, properties, and cardiotonic activity of
                        2-carbamovlmethylthio-6-phenyl-5-ethoxycarbonyl-3-
                        cyclo-4-(pyrido-3'yl)pyridine derivatives and their
                        hydrogenated analogs
AUTHOR(S):
                        Krauze, A.; Garalene, V.; Duburs, G.
CORPORATE SOURCE:
                        Inst. Org. Synth., Riga, Latvia
SOURCE:
                        Khimiko-Farmatsevticheskii Zhurnal (1992), 26(5), 40-3
                        CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        Russian
GT
/ Structure 55 in file .gra /
    Cyclocondensation of PhCOCH2CO2Et with 2-cvano-3-pyridinethioacrylamide in
```

AB Cyclocondensation of PhCOCH2CO2Et with 2-cyano-3-pyridinethioacrylamide in the presence of bases gave pyridinecarboxylates I (X+ = piperidino, Na) which when treated with ICH2CONH2 gave 82% amide II; betaine III (R = H) similarly treated gave amide III (R = CH2CONH2) which underwent base-catalyzed cyclization to give thienopyridine IV (RI = 3-pyridyl). Addnl. obtained was IV (RI = Ph). The 4,3'-bipyridines show dual activity-neg. inotropic action at low concns. and pos. inotropic activity at concns. >10-5M.

IT ***144969-93-7P***

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn., cyclization, and cardiotonic properties of)

RN 144969-93-7 CAPLUS

CN [3,4'-Bipyridine]-3'-carboxylic acid, 6'-[(2-amino-2-oxoethyl)thio]-5'cyano-2'-phenyl-, ethyl ester (CA INDEX NAME)

```
/ Structure 56 in file .gra /
```

L10 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:515227 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 113:115227

ORIGINAL REFERENCE NO.: 113:19527a,19530a

TITLE: Polycyclic pyridines. Part 8. Synthesis of new

primary, secondary and tertiary 3-aminothieno[2,3-b]pyridine-2-carboxamides by different pathways Wagner, G.; Vieweg, H.; Leistner, S.; Boehm, N.;

AUTHOR(S): Wagner, G.; Vieweg, H.; Leistner, S.; Boehm, N.; Krasselt, U.; Hanfeld, Vera; Prantz, J.; Grupe, Renate

CORPORATE SOURCE: Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010,

Ger. Dem. Rep.

SOURCE: Pharmazie (1990), 45(2), 102-9 CODEN: PHARAT: ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: German
OTHER SOURCE(S): CASREACT 113:115227

GI

/ Structure 57 in file .gra /

AB The treatment of 2-thioxo-1,2-dihydropyridine-3-carbonitriles with CICHZCOZNRIRS (RI, R2 = H, Me, Et) gave 3-aminothieno[2,3-b] b]pyridinecarboxylic acid amides I [RI = H, Et, Me; R2 = H, Et, Bu, cyclohexyl, CHZCHZOH, CHZCOZH; RIRZ = (CHZ)5; R3 = Me, Ph, 4-BrC6H4, 3-pyridyl, COMHZ, etc; R4 = H, Me, CHZC6H4(CN)-4; R5 = Me, C6H4C1-4, Ph, C6H4Br-4, furyl, naphthyl, OH). Some of the compds. thus prepd. e.g. I [RI = R2 = R4 = H, R3 = Me, R5 = Ph) and I (RI = R4 = H, R2 = CHZCHZOH, R3 = R5 = Me) showed activity as antiallergics in the passive cutaneous anaphylaxis test in rats.

IT ***127144-07-4***

RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with chloroacetamide)

RN 127144-07-4 CAPLUS

CN [3,4'-Bipyridine]-3'-carbonitrile, 1',2'-dihydro-6'-(2-naphthalenyl)-2'thioxo- (CA INDEX NAME)

/ Structure 58 in file .gra /

L10 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:216643 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 112:216643

ORIGINAL REFERENCE NO.: 112:36565a,36568a

TITLE: Multicyclic pyridines. Part 6. Synthesis of new

heterocycle substituted 2-thioxo-1, 2-dihydropyridine-3-

carbonitriles

AUTHOR(S): Vieweg, H.; Hanfeld, Vera; Leistner, S.; Wagner, G. CORPORATE SOURCE: Sekt. Biowiss., Karl-Marx-Univ., Leipzig, DDR-7010.

Ger. Dem. Rep.

SOURCE: Pharmazie (1989), 44(9), 639-40

CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 112:216643

GI

DM

/ Structure 59 in file .gra /

AB Condensation of RICOMe (RI = 2-furyl, 2-thienyl, 2-naphthyl) with RZCHO (R2 = Ph, 4-FC6H4, 4-ELC6H4, 4-BrCH4H, 3-pyridyl) in MeOH or HZO contg. NaOH gave 45-88% RICOCH:CHRZ which on cyclocondensation with NH2CSCH2CN in the presence of NaOMe in MeOH gave 32-71% title compds. I. Cyclocondensation of 1-(2-thienyl)-1,3-butanedione with NH2CSCH2CN in the presence of KZCO3-MeZCO gave isomeric mixt. of I (RI = 2-thienyl, RZ = Me; RI = Me, RZ = 2-thienyl) which on condensation with CLGUCOZET followed by base-mediated cyclization gave thienopyridinecarboxylates II (R3 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me, R4 = 2-thienyl, R4 = Me; R3 = Me; R4 =

IT ***127144-07-4P***
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of) 127144-07-4 CAPLUS

CN [3,4'-Bipyridine]-3'-carbonitrile, 1',2'-dihydro-6'-(2-naphthalenyl)-2'-thioxo- (CA INDEX NAME)

/ Structure 60 in file .gra /

=> file req

 COST IN U.S. DOLLARS
 SINCE FILE
 TOTAL

 FULL ESTIMATED COST
 30.13
 588.45

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL | ENTRY | SESSION | CA SUBSCRIBER PRICE | -4.00 | -6.40 |

FILE 'REGISTRY' ENTERED AT 11:52:49 ON 08 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1 DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting ${\tt SmartSELECT}$ searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Program Files\STNEXP\Queries\10542351 take 6.str

L11 STRUCTURE UPLOADED

=> d 111 L11 HAS NO ANSWERS

STR / Structure 61 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

Uploading C:\Program Files\STNEXP\Oueries\10542351 take 7.str

STRUCTURE UPLOADED T.12

=> d 112

L12 HAS NO ANSWERS L12 STR

/ Structure 62 in file .gra /

Structure attributes must be viewed using STN Express query preparation.

=> s 111 sss sam

SAMPLE SEARCH INITIATED 11:54:10 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2127 TO ITERATE

94.0% PROCESSED 2000 ITERATIONS 50 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS: 39774 TO 45306 PROJECTED ANSWERS: 38498 TO 43944

1.13 50 SEA SSS SAM L11

=> s 111 sss ful

FULL SEARCH INITIATED 11:54:24 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 41604 TO ITERATE

100.0% PROCESSED 41604 ITERATIONS

40140 ANSWERS

SEARCH TIME: 00.00.01

=> s 112 sss ful

FULL SEARCH INITIATED 11:55:00 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 51043 TO ITERATE

100.0% PROCESSED 51043 ITERATIONS

2250 ANSWERS

SEARCH TIME: 00.00.01

L15 2250 SEA SSS FUL L12

=> file cap

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 357.64 946.09

SINCE FILE TOTAL ENTRY SESSION DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) CA SUBSCRIBER PRICE 0.00 -6.40

FILE 'CAPLUS' ENTERED AT 11:55:04 ON 08 SEP 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11 FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> s 114 or 115 1101 L14

765 L15

1.16 1125 L14 OR L15

=> d 116 and bacteria

'AND' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

'BACTERIA' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB

```
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
CLASS ----- IPC, NCL, ECLA, FTERM
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
             SCAN must be entered on the same line as the DISPLAY,
             e.g., D SCAN or DISPLAY SCAN)
STD ---- BIB, CLASS
IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels
OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels
SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations
HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
            containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
             its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
             structure diagram, plus NTE and SEQ fields
FHITSTR ---- First HIT RN, its text modification, its CA index name, and
             its structure diagram
FHITSEO ---- First HIT RN, its text modification, its CA index name, its
            structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs
To display a particular field or fields, enter the display field
```

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

```
ENTER DISPLAY FORMAT (BIB):end
=> s 116 and bacteria
       348391 BACTERIA
          129 BACTERIAS
       348461 BACTERIA
                (BACTERIA OR BACTERIAS)
L17
           11 L16 AND BACTERIA
=> d scan
L17
    11 ANSWERS CAPLUS COPYRIGHT 2008 ACS on STN
    ICM C07D519-00
IC
ICA A61K031-545
ICI C07D519-00, C07D501-00, C07D495-00
    26-5 (Biomolecules and Their Synthetic Analogs)
    Section cross-reference(s): 1
TI
    Preparation of cephalosporin derivatives as antibacterial agents
ST
    thienopyridiniomethylcephemcarboxylate prepn antibacterial; cephalosporin
    prepn antibacterial; cephemcarboxylate thienopyridiniomethyl prepn
    antibacterial
TΤ
    Antibiotics
       ([thiazolyl(hydroxyimino)acetamido](thienopyridiniomethyl)cephemcarboxy
       late derivs.)
TΤ
    152938-71-1P
                 152938-72-2P
                                152938-73-3P
                                              152938-74-4P
                                                            152938-75-5P
    152938-76-6P
                 152938-77-7P 152938-78-8P 152938-79-9P 152938-80-2P
                                                            152938-85-7P
    152938-81-3P 152938-82-4P 152938-83-5P 152938-84-6P
    152938-86-8P 152938-87-9P 152938-88-0P 152938-89-1P
                                                             152938-90-4P
    152938-91-5P 152938-92-6P 152938-93-7P 152938-94-8P 152938-95-9P
    152938-96-0P
                 152938-97-1P 152938-98-2P 152938-99-3P 152939-00-9P
    152939-01-0P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); BIOL (Biological
    study); PREP (Preparation)
       (prepn. of, as antibacterial agent)
    151027-96-2P 151027-97-3P 152938-44-8P
                                              152938-45-9P
                                                            152938-46-0P
    152938-47-1P
                 152938-48-2P
                                152938-49-3P 152938-50-6P
                                                            152938-51-7P
    152938-52-8P 152938-53-9P 152938-54-0P 152938-55-1P 152938-56-2P
    152938-57-3P 152938-58-4P 152938-59-5P 152938-60-8P 152938-61-9P
    152938-62-0P 152938-63-1P 152938-64-2P
                                              152938-65-3P 152938-66-4P
    152938-67-5P 152938-68-6P 152938-69-7P
                                              152938-70-0P
                                                            152939-02-1P
                               152939-05-4P
                                              152939-06-5P
    152939-03-2P 152939-04-3P
                                                            152939-07-6P
    152939-08-7P 152939-09-8P 152939-10-1P
                                               ***152939-11-2P***
      ***152939-12-3P***
                         152939-13-4P 152939-14-5P, Thieno[2,3-
blpvridine-
    3.5-diamine 152939-15-6P 152939-16-7P 152939-17-8P 152939-18-9P
    152939-19-0P
                 152939-20-3P 152939-21-4P
                                              152939-22-5P 152939-23-6P
    152939-24-7P 152939-25-8P 152939-26-9P
                                              152939-27-0P
                                                            152939-28-1P
    152939-29-2P
                  152939-30-5P
                                152939-32-7P
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. of, as intermediate for antibacterial cephalosporin deriv.)
    75-52-5, Nitromethane, reactions 105-36-2, Ethyl bromoacetate
    407-25-0, Trifluoroacetic anhydride 563-41-7, Semicarbazide
    hydrochloride 762-49-2, 1-Bromo-2-fluoroethane 883-40-9,
```

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC

to view a specified Accession Number.

Diphenyldiazomethane 2365-48-2, Methyl thioglycolate 7664-41-7, Ammonia, reactions 18600-39-0, Cyclopropylamine hydrochloride 24424-99-5, Di-tert-butyl dicarbonate 26579-54-4, Thieno[2,3-b]pyridin-3-amine 31309-08-7 53174-99-5, 3-Formylthieno[2,3-b]pyridine 84728-65-4 142604-12-4 152939-31-6, Thieno[2,3-b]pyridin-3-ol 152939-33-8 RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, in prepn. of antibacterial cephalosporin deriv.) 1111-112-9D, Cephalosporin, derivs.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

(thienopyridiniomethyl-)

=> d 117 1-11 ibib abs hitstr

L17 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

RL: RCT (Reactant); RACT (Reactant or reagent)

ACCESSION NUMBER: 2008:526897 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 149:121710

TITLE: Virtual screening and experimental verification to

identify potential inhibitors of the ErmC

methyltransferase responsible for bacterial resistance

against macrolide antibiotics

AUTHOR(S): Feder, Marcin; Purta, Elzbieta; Koscinski, Lukasz;

Cubrilo, Sonja; Vlahovicek, Gordana Maravic; Bujnicki,

Janusz M.

CORPORATE SOURCE: Laboratory of Bioinformatics and Protein Engineering,

International Institute of Molecular and Cell Biology,

Warsaw, 02109, Pol.

SOURCE: ChemMedChem (2008), 3(2), 316-322 CODEN: CHEMGX; ISSN: 1860-7179

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

RN

Methyltransferases from the Erm family catalyze S-adenosyl-L-methioninedependent modification of a specific adenine residue in bacterial 23S rRNA, thereby conferring resistance to clin. important macrolide, lincosamide, and streptogramin B antibiotics. Thus, far, no inhibitors of these enzymes have been identified or designed that would effectively abolish the resistance in vivo. We used the crystal structure of ErmC' methyltransferase as a target for structure-based virtual screening of a database composed of 58679 lead-like compds. Among 77 compds. selected for exptl. validation (63 predicted to bind to the catalytic pocket and 14 compds. predicted to bind to the putative RNA binding site), we found several novel inhibitors that decrease the minimal inhibitory concn. of a macrolide antibiotic erythromycin toward an Escherichia coli strain that constitutively expresses ErmC'. Eight of them have IC50 values in the micromolar range. Anal. of docking models of the identified inhibitors suggests a novel strategy to develop potent and clin. useful inhibitors. ТТ ***285987-27-1***

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(ErmC' methyltransferase inhibitor; virtual screening and exptl. verification to identify potential inhibitors of BrmC methyltransferase responsible for bacterial resistance against macrolide antibiotics) 285987-27-1 CAPLUS

CN 3-Pvridinecarbonitrile, 4-methyl-2,6-bis[(4-methylphenyl)thio]- (CA INDEX

/ Structure 63 in file .gra /

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2007:436667 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 147:469291

TITLE: A convenient synthesis of some new

indeno[1,2-b]pyridines and indeno[1,2-b]thieno[3,2-e]pyridine derivatives with potential biological

activity

AUTHOR(S): E1-Ossaily, Yasser A.

CORPORATE SOURCE: Chemistry Department, Assiut University, Assiut, Egypt

SOURCE: Phosphorus, Sulfur and Silicon and the Related

Elements (2007), 182(5), 1109-1117 CODEN: PSSLEC; ISSN: 1042-6507

PUBLISHER: Taylor & Francis, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 147:469291

GI

/ Structure 64 in file .gra /

AB Heterocyclization of 1,3-indandione with arylidene cyanoacetamide, or arylideneindanone with cyanoacetamide afforded indenopyridinethione, which underwent cyclization with Et chloroacetate or chloroacetone to give indenothienopyridines. The alkylthioindenopyridines, underwent ring closure with sodium ethoxide to produce aminoindenothienopyridines, e.g., I. The indenothienopyridinecarbonitriles underwent heterocyclization with carbon disulfide in pyridine to give indenopyridintothienopyrimidines, e.g., II. Most of the synthesized compds. were screened in vitro for their antimicrobial activities against four species of "*bacteria** and six species of fungi using chloramphenicol and terbinafine as stds.

II ***351767-56.69*** ***952720-95-59*** ***952720-97-79***

IT ***311767-75-6P*** ***952720-95-5P*** **
952720-98-8P ***952720-99-9P***

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(prepn., antibacterial and antifungal activity of indenopyridines, indenothienopyridines, and indenopyridinthienopyrimidines starting from indandione or (arylidene)indandiones using heterocyclization as key step)

RN 311767-75-6 CAPLUS

CN 1H-Indeno[1,2-b]pyridine-3-carbonitrile, 2,5-dihydro-5-oxo-4-(2-thienyl)-2thioxo- (CA INDEX NAME)

```
RN
   952720-95-5 CAPLUS
    5H-Indeno[1,2-b]pvridine-3-carbonitrile, 2-[(cvanomethyl)thio]-5-oxo-4-(2-
     thienyl) - (CA INDEX NAME)
/ Structure 66 in file .gra /
    952720-97-7 CAPLUS
CN
     5H-Indeno[1,2-b]pyridine-3-carbonitrile, 5-oxo-2-[(2-oxo-2-
     phenylethyl)thio]-4-(2-thienyl)- (CA INDEX NAME)
/ Structure 67 in file .gra /
    952720-98-8 CAPLUS
   Acetamide, 2-[[3-cyano-5-oxo-4-(2-thieny1)-5H-indeno[1,2-b]pyridin-2-
    yl]thio]- (CA INDEX NAME)
/ Structure 68 in file .gra /
    952720-99-9 CAPLUS
    Acetamide, 2-[[3-cyano-5-oxo-4-(2-thienyl)-5H-indeno[1,2-b]pyridin-2-
    yl]thio]-N-(4-methoxyphenyl)- (CA INDEX NAME)
/ Structure 69 in file .gra /
тт
       ***952720-93-3P***
                             ***952720-94-4P***
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation)
        (prepn., antibacterial and antifungal activity of indenopyridines,
        indenothienopyridines, and indenopyridinothienopyrimidines starting
        from indandione or (arylidene) indandiones using heterocyclization as
        key step)
     952720-93-3 CAPLUS
RN
CN
    5H-Indeno[1,2-b]pyridine-3-carbonitrile, 2-(methylthio)-5-oxo-4-(2-
     thienvl) - (CA INDEX NAME)
/ Structure 70 in file .gra /
    952720-94-4 CAPLUS
    5H-Indeno[1,2-b]pyridine-3-carbonitrile, 2-(ethylthio)-5-oxo-4-(2-thienyl)-
       (CA INDEX NAME)
/ Structure 71 in file .gra /
       ***952720-96-6P***
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn., antibacterial and antifungal activity of indenopyridines,
        indenothienopyridines, and indenopyridinothienopyrimidines starting
        from indandione or (arylidene)indandiones using heterocyclization as
```

kev step)

```
RN
    952720-96-6 CAPLUS
CN
     Acetamide, N-(4-chlorophenyl)-2-[[3-cyano-5-oxo-4-(2-thienyl)-5H-
     indeno[1,2-b]pvridin-2-vl]thio]- (CA INDEX NAME)
/ Structure 72 in file .gra /
ΤТ
       ***952721-00-5P***
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn., antibacterial and antifungal activity of indenopyridines,
        indenothienopyridines, and indenopyridinothienopyrimidines starting
        from indandione or (arylidene)indandiones using heterocyclization as
        key step)
     952721-00-5 CAPLUS
CN
     5H-Indeno[1,2-b]pyridine-3-carbonitrile, 5-oxo-2-[(phenylmethyl)thio]-4-(2-
     thienyl) - (CA INDEX NAME)
/ Structure 73 in file .gra /
REFERENCE COUNT:
                        13
                              THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER.
                        2007:196524 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         147:419384
TITLE:
                         New antimicrobial 9-(p-heterocyclo-substituted
                         anilino)-tetrahydroacridines
AUTHOR(S):
                         Ebeid, M. Y.; Kamel, M. M.; Nofal, Z. M.; Ragab, F.;
                         Zaghary, W. A.; El-Kady, M.
                         Faculty of Pharmacy, Cairo University, Egypt
CORPORATE SOURCE:
SOURCE:
                         Egyptian Journal of Chemistry (2006), 49(2), 277-285
                         CODEN: EGJCA3; ISSN: 0449-2285
PUBLISHER:
                         National Information and Documentation Centre
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
     A new series of 9-[p-(4-arvl-3-cvano-2-iminopyridin-6-vl)anilino]-
     1,2,3,4-tetrahydroacridines and their 2-oxo-(or thioxo)-pyridinylanilino
     derivs. were synthesized and evaluated against ***bacteria***
     fungi. These compds. showed high significant activity against
     Saccharomyces cerevisiae, Bacillus subtilis, Staphylococcus aureus,
     Penicillium notatum, Aspergillus niger, Candida utilis, and Candida
     albicans.
       ***951320-46-0P***
     RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation)
        (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahvdroacridines)
RN
     951320-46-0 CAPLUS
CN
     3-Pyridinecarbonitrile, 1,2-dihydro-4-phenyl-6-[4-[(1,2,3,4-tetrahydro-9-
     acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 74 in file .gra /
ΙT
       ***951320-47-1P***
                            ***951320-48-2P***
                                                     ***951320-49-3P***
```

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

```
(new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahydroacridines)
RN
     951320-47-1 CAPLUS
CN
     3-Pyridinecarbonitrile, 1,2-dihydro-4-(3-methoxyphenyl)-6-[4-[(1,2,3,4-
     tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 75 in file .gra /
     951320-48-2 CAPLUS
CN
     3-Pyridinecarbonitrile, 4-(3-chlorophenyl)-1,2-dihydro-6-[4-[(1,2,3,4-
     tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 76 in file .gra /
     951320-49-3 CAPLUS
     3-Pyridinecarbonitrile, 1,2-dihydro-6-[4-[(1,2,3,4-tetrahydro-9-
     acridinvl)amino|phenvl]-2-thioxo-4-(2,3,4-trimethoxyphenvl)- (CA INDEX
     NAME)
/ Structure 77 in file .gra /
       ***951320-50-6***
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (new antimicrobial 9-(p-heterocyclo-substituted anilino)-
        tetrahydroacridines)
RM
     951320-50-6 CAPLUS
     3-Pyridinecarbonitrile, 4-[3-(dimethylamino)phenyl]-1,2-dihydro-6-[4-
CN
     [(1,2,3,4-tetrahydro-9-acridinyl)amino]phenyl]-2-thioxo- (CA INDEX NAME)
/ Structure 78 in file .gra /
                               THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                         20
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        2003:971725 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         140:35893
TITLE:
                         Transcription factor modulating compounds and methods
                         of use thereof
INVENTOR(S):
                         Levy, Stuart B.; Alekshun, Michael N.; Podlogar, Brent
                         L.; Ohemeng, Kwasi; Verma, Atul K.; Warchol, Tadeusz;
                         Bhatia, Beena
PATENT ASSIGNEE(S):
                         USA
SOURCE:
                         U.S. Pat. Appl. Publ., 301 pp.
                         CODEN: USXXCO
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:
     PATENT NO.
                        KIND
                                                                 DATE
                              DATE
                                           APPLICATION NO.
     US 20030229065
                        A1
                                                                  20020814
```

20031211

US 2002-139591

```
CA 2445515
                      A1 20021104 CA 2002-2445515
                                                            20020506
                             20031231 WO 2002-US14255
    WO 2004001058
                       A2
                                                             20020506
    WO 2004001058
                       A3
                             20050303
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
           GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
           GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
            GN, GQ, GW, ML, MR, NE, SN, TD, TG
                            20040106
                                        AU 2002-367953
    AU 2002367953
                       A1
    AU 2002367953
                       B2
                             20080717
    EP 1524974
                       A2
                            20050427 EP 2002-807554
                                                              20020506
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
    JP 2005519998
                       T
                            20050707 JP 2004-515557
                                                             20020506
    US 20050124678
                      A1
                            20050609
                                      US 2003-700661
                                                              20031103
    US 7405235
                      B2 20080729
    AU 2008203017
                      A1 20080731
                                        AU 2008-203017
                                                              20080708
                                                         P 20010504
                                        US 2001-288660P
PRIORITY APPLN. INFO.:
                                         AU 2002-367953
                                                          A3 20020506
                                         WO 2002-US14255
                                                          W 20020506
                                                          A2 20020814
                                         US 2002-139591
                                         US 2002-423319P
                                                          P 20021101
                                         US 2002-425916P P 20021113
                       MARPAT 140:35893
OTHER SOURCE(S):
```

AB Methods for identifying compd. useful as anti-infectives that decrease resistance, virulence, or growth of microbes are provided. In one embodiment, the method comprises contacting a microbial cell comprising: (1) a selectable marker under the control of a transcription factor responsive element and (2) a transcription factor, with a compd. under conditions which allow interaction of the compd. with the microbial cell; and measuring the ability of the compd. to affect the growth or survival of the microbial cell as an indication of whether the test compd. modulates the activity of a transcription factor.

IT ***221179-01-7*** ***299198-34-8***

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(transcription factor modulating compds. as anti-infectives agents that decrease resistance and virulence and growth identified by detg. marker under control of responsive element)

RN 221179-01-7 CAPLUS

CN 3,5-Pyridinedicarbonitrile, 2-amino-4-(4-hydroxyphenyl)-6-[[2-oxo-2-(2-oxo-2H-1-benzopyran-3-yl)ethyl]thio]- (CA INDEX NAME)

```
/ Structure 79 in file .gra /
```

RN 299198-34-8 CAPLUS

CN 3-Pyridinecarbonitrile, 2-[(2-cyclopropyl-2-oxoethyl)thio]-6-(2-thienyl)-4-(trifluoromethyl)- (CA INDEX NAME)

```
/ Structure 80 in file .gra /
```

L17 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:912358 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 139:381381

TITLE: Preparation of antibacterial pyridinedicarbonitriles

INVENTOR(S): Grant, Richard; Latham, Christopher J.; Thomson,

Samantha; Zhao, Lihua PATENT ASSIGNEE(S): Pantherix Ltd., UK

SOURCE: Brit. UK Pat. Appl., 18 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2388593	A	20031119	GB 2002-10898	20020513
PRIORITY APPLN. INFO.:			GB 2002-10898	20020513
OTHER SOURCE(S):	MARPAT	139:381381		
GI				

/ Structure 81 in file .gra /

The title compds. [I; n = 0-2; R1 = H, alkyl, CN, aryl, etc.] which have AB ***bacteria*** , were antibacterial activity, esp. against gram pos. prepd. Thus, reacting 2-amino-3,5-dicvano-6-mercaptopyridine with 2-chloro-N-(2,5-dimethylphenyl)acetamide in the presence of K2CO3 in DMF afforded 19% I [n = 0; R1 = 2,5-Me2C6H3] which showed IC50 in the range of 1-50 .mu.M against isolated Streptococcus pneumoniae chorismate synthase. Pharmaceutical compn. comprising the compd. I is claimed.

```
***298216-30-5P***
                      ***303065-59-0P***
                                            ***303065-61-4P***
***303065-63-6P***
                      ***311314-38-2P***
                                           ***311314-61-1P***
***311332-03-3P***
                      ***311789-13-6P***
                                           ***311795-13-8P***
***312318-88-0P***
                      ***312509-66-3P***
                                            ***312513-87-4P***
***312513-88-5P***
                      ***318258-92-3P***
                                            ***329206-96-4P***
***331421-74-0P***
                      ***331966-90-6P***
                                             ***331966-91-7P***
***331966-98-4P***
                      ***332114-15-5P***
                                             ***337918-65-7P***
                      ***337926-03-1P*** , Acetamide, N, N'-(9H-fluoren-
***337918-66-8P***
```

9vlidenedi-4,1-phenylene)bis[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-***339153-44-5P*** ***339576-16-8P*** ***339584-40-6P***

348146-19-0P ***348580-92-7P*** ***348581-11-3P*** ***356589-29-2P*** ***356589-40-7P*** ***356589-45-2P*** ***356589-52-1P*** ***356589-54-3P*** ***356589-62-3P*** ***356589-71-4P*** ***400864-06-4P*** ***625109-52-6P***

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of antibacterial pyridinedicarbonitriles) 298216-30-5 CAPLUS

RN

Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(2-cyanopheny1)-CN (CA INDEX NAME)

```
/ Structure 82 in file .gra /
RN 303065-59-0 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(2,6-
    dimethylphenyl) - (CA INDEX NAME)
/ Structure 83 in file .gra /
RN
   303065-61-4 CAPLUS
CN Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(2-methylpheny1)-
     (CA INDEX NAME)
/ Structure 84 in file .gra /
RN 303065-63-6 CAPLUS
CN Acetamide, 2-[(6-amino-3,5-dicvano-2-pvridinvl)thio]-N-(3-methylphenvl)-
    (CA INDEX NAME)
/ Structure 85 in file .gra /
    311314-38-2 CAPLUS
CN Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(2-bromopheny1)-
    (CA INDEX NAME)
/ Structure 86 in file .gra /
RN
    311314-61-1 CAPLUS
    Acetamide, N,N'-(3,3'-dimethoxy[1,1'-biphenyl]-4,4'-diyl)bis[2-[(6-amino-
     3,5-dicyano-2-pyridinyl)thio]- (9CI) (CA INDEX NAME)
/ Structure 87 in file .gra /
   311332-03-3 CAPLUS
RN
CN
   Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(3-methoxyphenyl)-
     (CA INDEX NAME)
/ Structure 88 in file .gra /
DM
   311789-13-6 CAPLUS
CN Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N,N-diphenyl- (CA
     INDEX NAME)
/ Structure 89 in file .gra /
RN
   311795-13-8 CAPLUS
CN Acetamide, 2-[(6-amino-3,5-dicvano-2-pyridinyl)thio]-N-[3-
     (trifluoromethyl)phenyl]- (CA INDEX NAME)
```

```
/ Structure 90 in file .gra /
    312318-88-0 CAPLUS
CN Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-butoxyphenyl)-
    (CA INDEX NAME)
/ Structure 91 in file .gra /
    312509-66-3 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(2,5-
    dimethylphenyl) - (CA INDEX NAME)
/ Structure 92 in file .gra /
    312513-87-4 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(2-ethoxypheny1)-
     (CA INDEX NAME)
/ Structure 93 in file .gra /
    312513-88-5 CAPLUS
CN
   Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(4-ethoxypheny1)-
    (CA INDEX NAME)
/ Structure 94 in file .gra /
    318258-92-3 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-phenyl- (CA INDEX
CN
    NAME)
/ Structure 95 in file .gra /
    329206-96-4 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicvano-2-pvridinvl)thio]-N-(4-bromophenvl)-
    (CA INDEX NAME)
/ Structure 96 in file .gra /
    331421-74-0 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-cyanophenyl)-
     (CA INDEX NAME)
/ Structure 97 in file .gra /
RN
    331966-90-6 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-methoxyphenyl)-
CN
     (CA INDEX NAME)
/ Structure 98 in file .gra /
```

```
RN
    331966-91-7 CAPLUS
     Acetamide, 2-[(6-amino-3,5-dicvano-2-pvridinvl)thio]-N-(2-methoxyphenvl)-
     (CA INDEX NAME)
/ Structure 99 in file .gra /
     331966-98-4 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicvano-2-pyridiny1)thio]-N-(2-fluoropheny1)-
     (CA INDEX NAME)
/ Structure 100 in file .gra /
     332114-15-5 CAPLUS
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-[4-
     (aminosulfonyl)phenyl]- (CA INDEX NAME)
/ Structure 101 in file .gra /
     337918-65-7 CAPLUS
    Acetamide, N,N'-1,4-phenylenebis[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-
       (CA INDEX NAME)
/ Structure 102 in file .gra /
RN
     337918-66-8 CAPLUS
     Acetamide, N, N'-(2-chloro-1, 4-phenylene) bis[2-[(6-amino-3, 5-dicyano-2-
     pyridinyl)thio]- (CA INDEX NAME)
/ Structure 103 in file .gra /
     337926-03-1 CAPLUS
CN
     Acetamide, N,N'-(9H-fluoren-9-ylidenedi-4,1-phenylene)bis[2-[(6-amino-3,5-
     dicvano-2-pyridinyl)thio|- (9CI) (CA INDEX NAME)
/ Structure 104 in file .gra /
     339153-44-5 CAPLUS
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(4-chloropheny1)-
     (CA INDEX NAME)
/ Structure 105 in file .gra /
     339576-16-8 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(4-methylphenyl)-
     (CA INDEX NAME)
/ Structure 106 in file .gra /
```

```
RN 339584-40-6 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridiny1)thio]-N-(4-methoxy-2-
    nitrophenvl) - (CA INDEX NAME)
/ Structure 107 in file .gra /
RN
    348146-19-0 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-[4-[(2-
CN
     thiazolvlamino)sulfonvl]phenvl]- (CA INDEX NAME)
/ Structure 108 in file .gra /
RN
    348580-92-7 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(3,4-
CN
    dichlorophenvl) - (CA INDEX NAME)
/ Structure 109 in file .gra /
    348581-11-3 CAPLUS
RN
    Acetamide, 2-((6-amino-3,5-dicvano-2-pyridinyl)thio|-N-(2,6-
CN
    dichlorophenyl) - (CA INDEX NAME)
/ Structure 110 in file .gra /
RM
    356589-29-2 CAPLUS
CN
    Acetamide, N-[4-(acetylamino)phenyl]-2-[(6-amino-3,5-dicyano-2-
    pyridinyl)thio]- (CA INDEX NAME)
/ Structure 111 in file .gra /
RN
    356589-40-7 CAPLUS
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-[4-
     (methylthio)phenyl]- (CA INDEX NAME)
/ Structure 112 in file .gra /
    356589-45-2 CAPLUS
RN
    Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(9,10-dihydro-9,10-
    dioxo-2-anthracenyl)- (CA INDEX NAME)
/ Structure 113 in file .gra /
RN
    356589-52-1 CAPLUS
CN
    Benzoic acid, 4-[[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]acetyl]amino]-
     (CA INDEX NAME)
/ Structure 114 in file .gra /
RN 356589-54-3 CAPLUS
```

```
(CA INDEX NAME)
/ Structure 115 in file .gra /
     356589-62-3 CAPLUS
CN
    Acetamide, 2-[(6-amino-3,5-dicvano-2-pyridinyl)thio]-N-[2-chloro-5-
     (trifluoromethyl)phenyl]- (CA INDEX NAME)
/ Structure 116 in file .gra /
     356589-71-4 CAPLUS
CN Benzoic acid, 5-[[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]acetyl]amino]-2-
     chloro- (CA INDEX NAME)
/ Structure 117 in file .gra /
     400864-06-4 CAPLUS
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-2-naphthalenyl-
CN
     (CA INDEX NAME)
/ Structure 118 in file .gra /
DM
     625109-52-6 CAPLUS
CN
     Acetamide, 2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]-N-(3,4-
     dimethylphenyl) - (CA INDEX NAME)
/ Structure 119 in file .gra /
TT
      ***111971-56-3***
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of antibacterial pyridinedicarbonitriles)
     111971-56-3 CAPLUS
CN
     3,5-Pvridinedicarbonitrile, 6-amino-1,2-dihvdro-2-thioxo- (CA INDEX NAME)
/ Structure 120 in file .gra /
REFERENCE COUNT:
                         2
                               THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         2003:145365 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                         139:270296
TITLE:
                         Novel 4-aminopyrimido[4,5-b]quinoline derivatives as
                         potential antimicrobial agents
AUTHOR(S):
                         El-Sayed, Ola A.; El-Bieh, Fatma M.; El-Aqeel, Shada
                         I.; Al-Bassam, Badr A.; Hussein, Maher E.
CORPORATE SOURCE:
                         Pharmaceutical Chemistry Department, Faculty of
                         Pharmacy, University of Alexandria, Alexandria, 21521,
                         Eavot.
SOURCE:
                         Bollettino Chimico Farmaceutico (2002), 141(6),
```

CN Benzoic acid, 3-[[2-[(6-amino-3,5-dicyano-2-pyridinyl)thio]acetyl]amino]-

461-465

CODEN: BCFAAI; ISSN: 0006-6648 Societa Editoriale Farmaceutica

DOCUMENT TYPE: Journal LANGUAGE: English

PUBLISHER:

/ Structure 121 in file .gra /

AR Two series of 4-aminopyrimido[4,5-b]quinoline derivs. substituted in the 2-position , e.g. I, and/or in 1-position, e.g. II, have been prepd. by facile routes starting from 2-amino-3-cyanoquinoline 2,2-chloro-3cyanoquinoline, and 2-arylamino-3-cyanoquinolines. The reactions involved simple fusion with thiourea or urea and, in some cases, with guanidine. The prepd. compds. were in vitro tested for antimicrobial activities against some selected Gram-pos., Gram-neg. ***bacteria*** and fungi. Products contg. the thio-function were the most active followed by those contg. the imino-function while the carbonyl contg. derivs. were without significant antimicrobial effect.

69513-35-5P IΤ

> RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and properties of)

RN 69513-35-5 CAPLUS

AUTHOR(S):

CORPORATE SOURCE:

CN 3-Quinolinecarbonitrile, 1,2-dihydro-2-thioxo- (CA INDEX NAME)

/ Structure 122 in file .gra /

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:221628 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 130:325083

TITLE: Synthesis and antimicrobial activity of some new

4-methylquinolines Kamel, M. M.; Fathala, O. A.; Abdou, W. A. M.; Haiba,

M. E.

Medicinal Chemistry Department, National Research

Centre, Cairo, Egypt Proceedings of the Pakistan Academy of Sciences

SOURCE:

(1997), 34(1), 7-11

CODEN: PKSPAW: ISSN: 0377-2969

Pakistan Academy of Sciences

PUBLISHER: DOCUMENT TYPE: Journal

LANGUAGE: English

Some new 4,8-dimethyl-2-[p-(3-cyano-2-thioxo-4-arylpyridine-6-

yl)]anilinoquinolines and 7-chloro-4-methyl-2-(4-hydroxy)anilinoquinoline Mannich bases were synthesized for the purpose of antimicrobial evaluation against ***bacteria*** , yeast, and fungi. Two compds. showed activity against these microorganisms.

TT ***218272-67-4P*** ***218272-68-5P*** ***218272-69-6P***

218272-70-9P ***223697-02-7P***

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

```
BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. of methylquinolines as antibacterial and antifungal agents)
RN
     218272-67-4 CAPLUS
CN
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 123 in file .gra /
     218272-68-5 CAPLUS
CN
     3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-6-[4-[(4,8-dimethyl-2-
     quinolinyl)amino]phenyl]-1,2-dihydro-2-thioxo- (CA INDEX NAME)
/ Structure 124 in file .gra /
     218272-69-6 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(3-methoxy-2-nitrophenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 125 in file .gra /
     218272-70-9 CAPLUS
CN
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(2-thienyl)-2-thioxo- (CA INDEX NAME)
/ Structure 126 in file .gra /
     223697-02-7 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(7-chloro-4-methyl-2-
     quinolinyl)amino]phenyl]-1,2-dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA
     INDEX NAME)
/ Structure 127 in file .gra /
REFERENCE COUNT:
                         17
                               THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
                               RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
                        1998:702455 CAPLUS <<LOGINID::20080908>>
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         130:66375
TITLE:
                         Synthesis of some new 4-methylquinolines of possible
                         biological activity
AUTHOR(S):
                         Kamel, M. M.; Fathalla, O. A.; Abdou, W. A. M.; Omer,
                         M. T.; Haiba, M. E.
CORPORATE SOURCE:
                         Medicinal Chemistry Department, National Research
                         Centre, Cairo, Egypt
SOURCE:
                         Egyptian Journal of Pharmaceutical Sciences (1998),
                         Volume Date 1997, 38(1-3), 79-86
                         CODEN: EJPSBZ; ISSN: 0301-5068
PUBLISHER:
                         National Information and Documentation Centre
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
AB Some new 4,8-dimethyl-2-[p-(3-cvano-2-thioxo-4-arylpyridin-6-
```

```
yl)]anilinoquinolines and 7-chloro-4-methyl-2-(4-hydroxy)anilinoquinolines
     Mannich bases were synthesized for the purpose of antimicrobial evaluation
     against ***bacteria*** , yeast, and fungi. 7-Chloro-4-methyl-2-[4-
     hydroxy-3,5-di(diethylaminomethyl) lanilinoquinoline showed fungicidal
     activity against Aspergillus niger.
       ***218272-67-4P***
                             ***218272-68-5P***
                                                   ***218272-69-6P***
       ***218272-70-9P***
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis and antimicrobial activity of 4-methylquinolines)
     218272-67-4 CAPLUS
     3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(4-methoxyphenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 128 in file .gra /
     218272-68-5 CAPLUS
    3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-6-[4-[(4,8-dimethyl-2-
     quinolinyl)amino]phenyl]-1,2-dihydro-2-thioxo- (CA INDEX NAME)
/ Structure 129 in file .gra /
     218272-69-6 CAPLUS
    3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(3-methoxy-2-nitrophenyl)-2-thioxo- (CA INDEX NAME)
/ Structure 130 in file .gra /
     218272-70-9 CAPLUS
    3-Pyridinecarbonitrile, 6-[4-[(4,8-dimethyl-2-quinolinyl)amino]phenyl]-1,2-
     dihydro-4-(2-thienyl)-2-thioxo- (CA INDEX NAME)
/ Structure 131 in file .gra /
                              THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
REFERENCE COUNT:
                        15
                               RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1998:702449 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                        130:81446
TITLE:
                        Synthesis of some new indole derivatives of possible
                        antimicrobial activity
AUTHOR(S):
                        Fahmy, H. H.; Kassem, E. M. M.; Abdou, W. A. M.;
                        Mahmoud, S. A.
CORPORATE SOURCE:
                        Department of Medicinal Chemistry, National Research
```

RN

CN

CN

SOURCE:

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE: English AB A series of indolyl arylidene hydrazones, indolylamidothiazolidin-4-ones, pyrazoline and pyrazolidindione derivs., 3-(3-cvano-4-aryl-2-imino-(1H)-

Volume Date 1997, 38(1-3), 13-22 CODEN: EJPSBZ; ISSN: 0301-5068

Egyptian Journal of Pharmaceutical Sciences (1998),

National Information and Documentation Centre

Centre, Cairo, Egypt

Journal

```
pyridin-6-yl)-indoles and 3-(3-cyano-4-aryl-2-thioxo-(1H)-pyridin-6-yl)-
     indoles were synthesized. Some of the new compds. showed considerable
     antimicrobial activity against gram + ve ***bacteria*** , yeast and
     fungi.
ΙT
       ***218784-55-5P***
                             ***218784-56-6P***
                                                   ***218784-57-7P***
       ***218784-58-8P***
                             ***218784-59-9P***
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (synthesis of new indole derivs. of possible antimicrobial activity)
RN
     218784-55-5 CAPLUS
    3-Pvridinecarbonitrile, 1,2-dihvdro-6-(1H-indol-3-v1)-4-phenvl-2-thioxo-
CN
     (CA INDEX NAME)
/ Structure 132 in file .gra /
     218784-56-6 CAPLUS
    3-Pvridinecarbonitrile, 1,2-dihvdro-6-(1H-indol-3-v1)-4-(4-methoxyphenv1)-
     2-thioxo- (CA INDEX NAME)
/ Structure 133 in file .gra /
    218784-57-7 CAPLUS
    3-Pyridinecarbonitrile, 4-(4-chlorophenyl)-1,2-dihydro-6-(1H-indol-3-yl)-2-
     thioxo- (CA INDEX NAME)
/ Structure 134 in file .gra /
     218784-58-8 CAPLUS
RN
    3-Pyridinecarbonitrile, 4-[4-(dimethylamino)phenyl]-1,2-dihydro-6-(1H-
     indol-3-v1)-2-thioxo- (CA INDEX NAME)
/ Structure 135 in file .gra /
    218784-59-9 CAPLUS
RN
CN
    3-Pyridinecarbonitrile, 1,2-dihydro-6-(1H-indol-3-yl)-2-thioxo-4-(3,4,5-
     trimethoxyphenyl) - (CA INDEX NAME)
/ Structure 136 in file .gra /
REFERENCE COUNT:
                        16
                              THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
                              RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT
L17 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                        1994:134144 CAPLUS <<LOGINID::20080908>>
DOCUMENT NUMBER:
                        120:134144
ORIGINAL REFERENCE NO.: 120:23615a,23618a
TITLE:
                        Preparation of cephalosporin derivatives as
                        antibacterial agents
INVENTOR(S):
                        Tanaka, Kyoshi; Sutani, Mineichi; Komatsu, Miwako;
                        Tsuchida, Keiichi; Saito, Akito; Hayashi, Kazuya;
                         Kanna, Hiroshi; Yonezawa, Kenji; Minami, Shinzaburo;
```

Watanabe, Yasuo

PATENT ASSIGNEE(S): Toyama Chemical Co Ltd, Japan SOURCE: Jpn. Kokai Tokkvo Koho, 26 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPL	ICATION NO.		DATE
					-	
JP 05202065	A	19930810	JP 19	991-311552		19911031
JP 05262777	A	19931012	JP 19	991-343936		19911202
JP 3141041	B2	20010305				
PRIORITY APPLN. INFO.:			JP 19	991-311552	Α1	19911031
OTHER SOURCE(S):	MARPAT	120:134144				
GI						

/ Structure 137 in file .gra /

- AR The title .beta.-lactams [I; R1 = (un)protected NH2; R2 = (cvano-, carbamoyl-, or halo-substituted) alkyl, alkenyl, alkynyl, or cycloalkyl; R3 = (un)protected CO2H, CO2-; R4 = H, (un)protected NH2; A = CH, CX; X = halo; B = bond, CH2NH, alkylene or O-lower alkylene optionally substituted with (un)protected hydroxy; D = NR5R6; R5 = H, H2N-protecting group; R6 = H, (cyano-, carbamoyl-, or halo-substituted) alkyl, alkenyl, aryl, or cycloalkyl; B-D = (halo)alkoxy; n = 0,1], having potent antibacterial ***bacteria*** including activity against gram pos. methicillin-resistant Staphylococcus aureus strains, are prepd. Thus, quaternization of 3-tert-butoxylcarbonylaminothieno[2,3-b]pyridine by p-methoxybenzyl 3-iodomethyl-7-[(Z)-2-methoxyimino-2-(2-tritylaminothiazol-4-yl)acetamido]-3-cephem-4-carboxylate in DMF at room temp. followed by deprotection with CF3CO2H in anisole gave 7-[2-(2-aminothiazol-4-yl)-(Z)-2methoxyiminoacetamido]-3-(3-amino-7-thieno[2,3-b]pyridinio)methyl-3-cephem-4-carboxylate (II). II showed min. inhibitory concn. of 1.56, 12.5, .ltoreq.0.1, and 1.56 .mu.q/mL against .beta.-lactamase-producing Staphylococcus aureus F-137, methicillin-resistant S. aureus F-597, Escherichia coli NIHJ JC-2, and Pseudomonas aeruginosa IFO 3445, resp. A total of 32 I were prepd.
- IT ***152939-11-2P*** ***152939-12-3P***
 - RL: SPN (Synthetic preparation); PREP (Preparation)
- (prepn. of, as intermediate for antibacterial cephalosporin deriv.) RN 152939-11-2 CAPLUS
- RN 152939-11-2 CAPLUS CN Acetic acid, 2-1(3-
- CN Acetic acid, 2-[(3-cyano-5-nitro-2-pyridinyl)thio]-, methyl ester (CA INDEX NAME)

```
/ Structure 138 in file .gra /
```

- RN 152939-12-3 CAPLUS
- CN Acetic acid, 2-[(5-amino-3-cyano-2-pyridinyl)thio]-, methyl ester (CA INDEX NAME)

```
/ Structure 139 in file .gra /
```

L17 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:514821 CAPLUS <<LOGINID::20080908>>

DOCUMENT NUMBER: 105:114821

ORIGINAL REFERENCE NO.: 105:18579a,18582a

TITLE: 2-(2-Aminothiazol-4-yl)-2-alkoxyiminoacetic acid

derivatives substituted on the oxime

INVENTOR(S): Heymes, Rene; Vignau, Michel

PATENT ASSIGNEE(S): Roussel-UCLAF , Fr.

SOURCE: Fr. Demande, 66 pp. Addn. to Fr. Demande Appl. No. 78

09617. CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	API	PLICATION NO.		DATE
FR 2553770	A2	19850426	FR	1983-16698	_	19831020
FR 2553770	B2	19860314				
FR 2438050	A2	19800430	FR	1978-24563		19780824
FR 2438050	B2	19830415				
AT 8100043	A	19821115	AT	1981-43		19810108
AT 371472	В	19830627				
US 4439433	A	19840327	US	1981-267638		19810527
GB 2101117	A	19830112	GB	1981-34540		19811117
GB 2101117	В	19830602				
CH 642648	A5	19840430	CH	1983-1949		19830411
PRIORITY APPLN. INFO.:			FR	1978-24563		19780824
			FR	1978-9617	A	19780331
			AT	1979-2403	A	19790330
			CH	1979-3008	A	19790330
			GB	1979-11275	A	19790330
				1979-25666	A3	19790330

OTHER SOURCE(S): CASREACT 105:114821; MARPAT 105:114821

GI

/ Structure 140 in file .gra /

AB 2-(2-Aminothiazol-4-yl)-2-alkoxyiminoacetic acid derivs. I [R = CXR2 (X = 0, 5; R2 = alkyl, alkoxy, Ph, substituted amino, substituted carboxyl, etc.,); R1 = C1, OMe, alkyl, cycloalkyl, alkylthio, acetoxymethyl, carbamoyloxymethyl, etc.; A = H, alk. metal, alk. earth metal, etc.], having good activity against gram-pos. ***bacteria*** (for example, the MIC for penicillin-resistant Staphylococcus was 1 .mu.g/ml after 24 and 48 h), are prepd. Thus, syn-2-(2-bromeethoxy)iminol-2-(2-tritylaminothiazol-4-yl)acetic acid [prepd. in 2 steps from Et 2-hydroxyimino-2-(2-tritylamino-4-thiazolyl)acetate-HCl] was acylated with tert-Bu 7-aminocephalosporanate to give tert-Bu 3-acetoxymethyl-7-[[2-(2-tritylaminothiazol-4-yl)-2-[2-bromoethoxy) imino]acetyl]aminolcebh-3-em-4-carboxylate (II). II was then deprotected and converted to the trifluoroacetate of syn-3-acetoxymethyl-7-[[2-(2-aminothiazol-4-yl)-2-[(2-bromoethoxy) imino]acetyl]aminolcebh-3-em-4-carboxylic acid.

```
тт
      ***72697-85-9P***
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and deblocking of)
RN
     72697-85-9 CAPLUS
CN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
     3-[(acetyloxy)methyl]-7-[[[[2-[(3-cyano-6-methyl-2-
     pvridinvl)thio|ethoxv|imino|[2-[(triphenvlmethvl)amino]-4-
     thiazolyl]acetyl]amino]-8-oxo-, [6R-[6.alpha.,7.beta.(Z)]]- (9CI) (CA
     INDEX NAME)
Absolute stereochemistry.
Double bond geometry as shown.
/ Structure 141 in file .gra /
       ***72697-31-5P***
                            ***72697-32-6P***
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (prepn. of, as antibiotic)
DΝ
     72697-31-5 CAPLUS
CN
     5-Thia-1-azabicvclo[4.2.0]oct-2-ene-2-carboxvlic acid,
     3-[(acetyloxy)methyl]-7-[[(2-amino-4-thiazolyl)][[2-[(3-cyano-6-methyl-2-
     pyridinyl)thio]ethoxy]imino]acetyl]amino]-8-oxo-, [6R-
     [6.alpha., 7.beta.(Z)]]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
Double bond geometry as shown.
/ Structure 142 in file .gra /
    72697-32-6 CAPLUS
RN
CN
     5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid,
     3-[(acetyloxy)methyl]-7-[[(2-amino-4-thiazolyl)][[2-[(3-cyano-6-methyl-2-
     pyridinyl)thio]ethoxy]imino]acetyl]amino]-8-oxo-, monosodium salt,
     [6R-[6.alpha., 7.beta.(Z)]]- (9CI) (CA INDEX NAME)
Absolute stereochemistry.
Double bond geometry as shown.
/ Structure 143 in file .gra /
=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:v
COST IN U.S. DOLLARS
                                                 SINCE FILE
                                                                 TOTAL
                                                      ENTRY
                                                              SESSION
FULL ESTIMATED COST
                                                      69.27
                                                               1015.36
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
                                                 SINCE FILE
                                                                TOTAL.
                                                      ENTRY
                                                               SESSION
CA SUBSCRIBER PRICE
                                                       -8.80
                                                                 -15.20
```

STN INTERNATIONAL LOGOFF AT 12:04:00 ON 08 SEP 2008